Numerical Python

Contents

- Efficient array computing in Python
- Creating arrays
- Indexing/slicing arrays
- Random numbers
- Linear algebra
- Plotting

More info

- Ch. 4 in the course book
- www.scipy.org
- The NumPy manual
- The SciPy tutorial

Numerical Python (NumPy)

- NumPy enables efficient numerical computing in Python
- NumPy is a package of modules, which offers efficient arrays (contiguous storage) with associated array operations coded in C or Fortran
- There are three implementations of Numerical Python
  - Numeric from the mid 90s (still widely used)
  - numarray from about 2000
  - numpy from 2006
- We recommend to use numpy (by Travis Oliphant)

```
from numpy import *
```

A taste of NumPy: a least-squares procedure

```
x = linspace(0.0, 1.0, n)                        # coordinates
y_line = -2*x + 3
y = y_line + random.normal(0, 0.25, n)  # line with noise

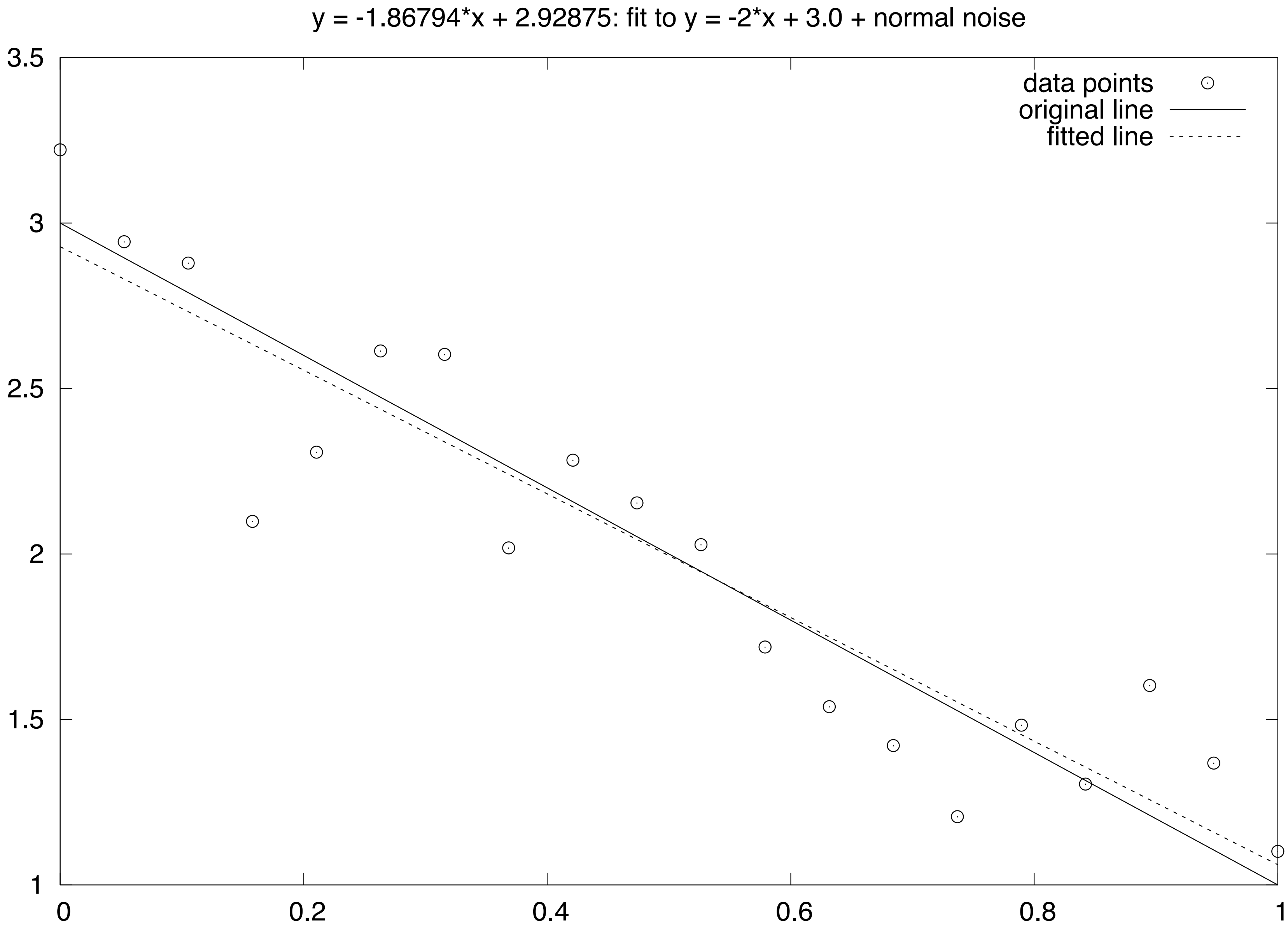
# goal: fit a line to the data points x, y

# create and solve least squares system:
A = array([x, ones(n)])
A = A.transpose()

result = linalg.lstsq(A, y)
# result is a 4-tuple, the solution (a,b) is the 1st entry:
a, b = result[0]

plot(x, y, 'o',          # data points w/noise
     x, y_line, 'r',     # original line
     x, a*x + b, 'b')    # fitted lines
legend('data points', 'original line', 'fitted line')
hardcopy('myplot.png')
```

Resulting plot



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Making arrays

```
>>> from numpy import *
>>> n = 4
>>> a = zeros(n)        # one-dim. array of length n
>>> print a
[ 0.  0.  0.  0.]
>>> a
array([ 0.,  0.,  0.,  0.])
>>> p = q = 2
>>> a = zeros((p,q,3))      # p*q*3 three-dim. array
>>> print a
[[[ 0.  0.  0.]
  [ 0.  0.  0.]]

 [[ 0.  0.  0.]
  [ 0.  0.  0.]]]
>>> a.shape                 # a's dimension
(2, 2, 3)
```

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Making float, int, complex arrays

```
>>> a = zeros(3)
>>> print a.dtype # a's data type
float64
>>> a = zeros(3, int)
>>> print a
[0 0 0]
>>> print a.dtype
int32
>>> a = zeros(3, float32)   # single precision
>>> print a
[ 0.  0.  0.]
>>> print a.dtype
float32
>>> a = zeros(3, complex)
>>> a
array([ 0.+0.j,  0.+0.j,  0.+0.j])
>>> a.dtype
dtype('complex128')

>>> given an array a, make a new array of same dimension
>>> and data type:
>>> x = zeros(a.shape, a.dtype)
```

Array with a sequence of numbers

- `linspace(a, b, n)` generates `n` uniformly spaced coordinates, starting with `a` and ending with `b`

```
>>> x = linspace(-5, 5, 11)
>>> print x
[-5. -4. -3. -2. -1.  0.  1.  2.  3.  4.  5.]
```

- A special compact syntax is also available:

```
>>> a = r_[-5:5:11j]  # same as linspace(-5, 5, 11)
>>> print a
[-5. -4. -3. -2. -1.  0.  1.  2.  3.  4.  5.]
```

- `arange` works like `range` (`xrange`)

```
>>> x = arange(-5, 5, 1, float)
>>> print x  # upper limit 5 is not included!!
[-5. -4. -3. -2. -1.  0.  1.  2.  3.  4.]
```

Warning: arange is dangerous

- `arange`'s upper limit may or may not be included (due to round-off errors)
- Better to use a safer method: `seq(start, stop, increment)`

```
>>> from scitools.numpyutils import seq
>>> x = seq(-5, 5, 1)
>>> print x    # upper limit always included
[-5. -4. -3. -2. -1.  0.  1.  2.  3.  4.  5.]
```

- The package `scitools` is available at `http://code.google.com/p/scitools/`

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Array construction from a Python list

- `array(list, [datatype])` generates an array from a list:

```
>>> pl = [0, 1.2, 4, -9.1, 5, 8]
>>> a = array(pl)
```

- The array elements are of the simplest possible type:

```
>>> z = array([1, 2, 3])
>>> print z                          # array of integers
[1 2 3]
>>> z = array([1, 2, 3], float)
>>> print z
[ 1.  2.  3.]
```

- A two-dim. array from two one-dim. lists:

```
>>> x = [0, 0.5, 1]; y = [-6.1, -2, 1.2]  # Python lists
>>> a = array([x, y])  # form array with x and y as rows
```

- From array to list: `alist = a.tolist()`

From “anything” to a NumPy array

- Given an object a,

```
a = asarray(a)
```

  converts a to a NumPy array (if possible/necessary)

- Arrays can be ordered as in C (default) or Fortran:

```
a = asarray(a, order='Fortran')
isfortran(a)  # returns True if a's order is Fortran
```

- Use asarray to, e.g., allow flexible arguments in functions:

```
def myfunc(some_sequence):
    a = asarray(some_sequence)
    return 3*a - 5

myfunc([1,2,3])        # list argument
myfunc((-1,1))         # tuple argument
myfunc(zeros(10))      # array argument
myfunc(-4.5)           # float argument
myfunc(6)              # int argument
```

Changing array dimensions

```
>>> a = array([0, 1.2, 4, -9.1, 5, 8])
>>> a.shape = (2,3)        # turn a into a 2x3 matrix
>>> print a
[[ 0.   1.2  4. ]
 [-9.1  5.   8. ]]
>>> a.size
6
>>> a.shape = (a.size,)    # turn a into a vector of length 6 agair
>>> a.shape
(6,)
>>> print a
[ 0.   1.2  4.  -9.1  5.   8. ]
>>> a = a.reshape(2,3)     # same effect as setting a.shape
>>> a.shape
(2, 3)
```

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Array initialization from a Python function

```
>>> def myfunc(i, j):
...     return (i+1)*(j+4-i)
...
>>> # make 3x6 array where a[i,j] = myfunc(i,j):
>>> a = fromfunction(myfunc, (3,6))
>>> a
array([[  4.,   5.,   6.,   7.,   8.,   9.],
       [  6.,   8.,  10.,  12.,  14.,  16.],
       [  6.,   9.,  12.,  15.,  18.,  21.]])
```

Basic array indexing

Note: all integer indices in Python start at 0!

```
a = linspace(-1, 1, 6)
a[2:4] = -1          # set a[2] and a[3] equal to -1
a[-1]  = a[0]        # set last element equal to first one
a[:]   = 0           # set all elements of a equal to 0
a.fill(0)            # set all elements of a equal to 0

a.shape = (2,3)      # turn a into a 2x3 matrix
print a[0,1]         # print element (0,1)
a[i,j] = 10          # assignment to element (i,j)
a[i][j] = 10         # equivalent syntax (slower)
print a[:,k]         # print column with index k
print a[1,:]         # print second row
a[:,:] = 0           # set all elements of a equal to 0
```

More advanced array indexing

```
>>> a = linspace(0, 29, 30)
>>> a.shape = (5,6)
>>> a
array([[  0.,   1.,   2.,   3.,   4.,   5.,]
       [  6.,   7.,   8.,   9.,  10.,  11.,]
       [ 12.,  13.,  14.,  15.,  16.,  17.,]
       [ 18.,  19.,  20.,  21.,  22.,  23.,]
       [ 24.,  25.,  26.,  27.,  28.,  29.,]])

>>> a[1:3,::2]   # a[i,j] for i=1,2 and j=0,2,4
array([[  6.,   8.,  10.],
       [ 12.,  14.,  16.]])

>>> a[::3,2::2]   # a[i,j] for i=0,3 and j=2,4
array([[  2.,   4.],
       [ 20.,  22.]])

>>> i = slice(None, None, 3);  j = slice(2, None, 2)
>>> a[i,j]
array([[  2.,   4.],
       [ 20.,  22.]])
```

Slices refer the array data

- With a as list, `a[:]` makes a copy of the data
- With a as array, `a[:]` is a reference to the data

```
>>> b = a[2,:]         # extract 2nd row of a
>>> print a[2,0]
12.0
>>> b[0] = 2
>>> print a[2,0]
2.0                    # change in b is reflected in a!
```

- Take a copy to avoid referencing via slices:

```
>>> b = a[2,:].copy()
>>> print a[2,0]
12.0
>>> b[0] = 2        # b and a are two different arrays now
>>> print a[2,0]
12.0                # a is not affected by change in b
```

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Loops over arrays (1)

- Standard loop over each element:

```
for i in xrange(a.shape[0]):
    for j in xrange(a.shape[1]):
        a[i,j] = (i+1)*(j+1)*(j+2)
        print 'a[%d,%d]=%g ' % (i,j,a[i,j]),
    print  # newline after each row
```

- A standard for loop iterates over the first index:

```
>>> print a
[[  2.   6.  12.]
 [  4.  12.  24.]]
>>> for e in a:
...     print e
...
[  2.   6.  12.]
[  4.  12.  24.]
```

Loops over arrays (2)

- View array as one-dimensional and iterate over all elements:

```
for e in a.ravel():
    print e
```

  Use `ravel()` only when reading elements, for assigning it is better to use `shape` or `reshape` first!

- For loop over all index tuples and values:

```
>>> for index, value in ndenumerate(a):
...     print index, value
...
(0, 0) 2.0
(0, 1) 6.0
(0, 2) 12.0
(1, 0) 4.0
(1, 1) 12.0
(1, 2) 24.0
```

Array computations

- Arithmetic operations can be used with arrays:

  ```
  b = 3*a - 1     # a is array, b becomes array
  ```

  1) compute `t1 = 3*a`, 2) compute `t2= t1 - 1`, 3) set `b = t2`

- Array operations are much faster than element-wise operations:

  ```
  >>> import time  # module for measuring CPU time
  >>> a = linspace(0, 1, 1E+07)  # create some array
  >>> t0 = time.clock()
  >>> b = 3*a -1
  >>> t1 = time.clock()   # t1-t0 is the CPU time of 3*a-1

  >>> for i in xrange(a.size): b[i] = 3*a[i] - 1
  >>> t2 = time.clock()
  >>> print '3*a-1: %g sec, loop: %g sec' % (t1-t0, t2-t1)
  3*a-1: 2.09 sec, loop: 31.27 sec
  ```

Standard math functions can take array arguments

```
# let b be an array

c = sin(b)
c = arcsin(c)
c = sinh(b)
# same functions for the cos and tan families

c = b**2.5  # power function
c = log(b)
c = exp(b)
c = sqrt(b)
```

Other useful array operations

```
# a is an array

a.clip(min=3, max=12)  # clip elements
a.mean(); mean(a)      # mean value
a.var();  var(a)       # variance
a.std();  std(a)       # standard deviation
median(a)
cov(x,y)               # covariance
trapz(a)               # Trapezoidal integration
diff(a)                # finite differences (da/dx)

# more Matlab-like functions:
corrcoeff, cumprod, diag, eig, eye, fliplr, flipud, max, min,
prod, ptp, rot90, squeeze, sum, svd, tri, tril, triu
```

More useful array methods and attributes

```
>>> a = zeros(4) + 3
>>> a
array([ 3.,  3.,  3.,  3.])  # float data
>>> a.item(2)                # more efficient than a[2]
3.0
>>> a.itemset(3,-4.5)        # more efficient than a[3]=-4.5
>>> a
array([ 3. ,  3. ,  3. , -4.5])
>>> a.shape = (2,2)
>>> a
array([[ 3. ,  3. ],
       [ 3. , -4.5]])
>>> a.ravel()                # from multi-dim to one-dim
array([ 3. ,  3. ,  3. , -4.5])
>>> a.ndim                   # no of dimensions
2
>>> len(a.shape)             # no of dimensions
2
>>> rank(a)                  # no of dimensions
2
>>> a.size                   # total no of elements
4
>>> b = a.astype(int)        # change data type
>>> b
array([3, 3, 3, 3])
```

Modules for curve plotting and 2D/3D visualization

- Matplotlib (curve plotting, 2D scalar and vector fields)
- PyX (PostScript/TeX-like drawing)
- Interface to Gnuplot
- Interface to Vtk
- Interface to OpenDX
- Interface to IDL
- Interface to Grace
- Interface to Matlab
- Interface to R
- Interface to Blender

Curve plotting with Easyviz

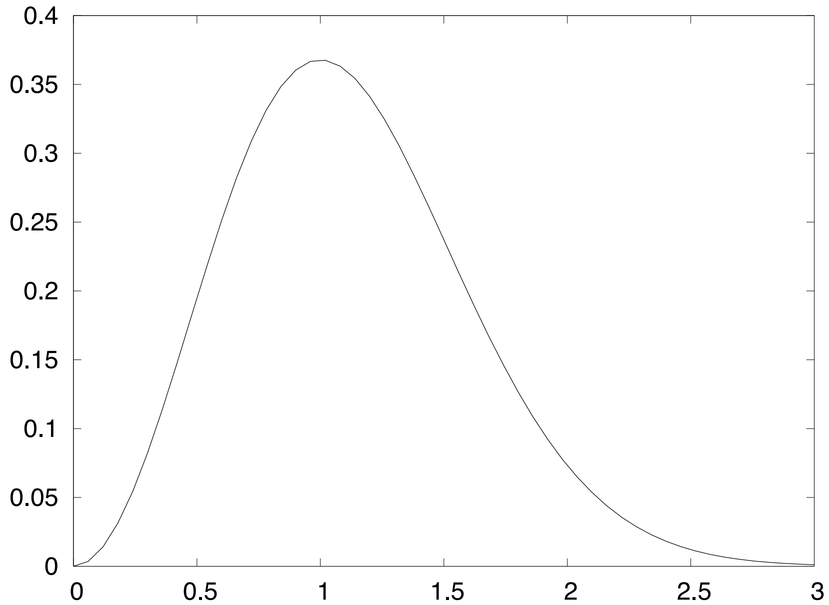
- Easyviz is a light-weight interface to many plotting packages, using a Matlab-like syntax
- Goal: write your program using Easyviz ("Matlab") syntax and postpone your choice of plotting package
- Note: some powerful plotting packages (Vtk, R, matplotlib, ...) may be troublesome to install, while Gnuplot is easily installed on all platforms
- Easyviz supports (only) the most common plotting commands
- Easyviz is part of SciTools (Simula development)

  ```
  from scitools.all import *
  ```

  (imports all of `numpy`, all of `easyviz`, plus `scitools`)

Basic Easyviz example

```
from scitools.all import *  # import numpy and plotting
t = linspace(0, 3, 51)      # 51 points between 0 and 3
y = t**2*exp(-t**2)         # vectorized expression
plot(t, y)
hardcopy('tmp1.eps')  # make PostScript image for reports
hardcopy('tmp1.png')  # make PNG image for web pages
```



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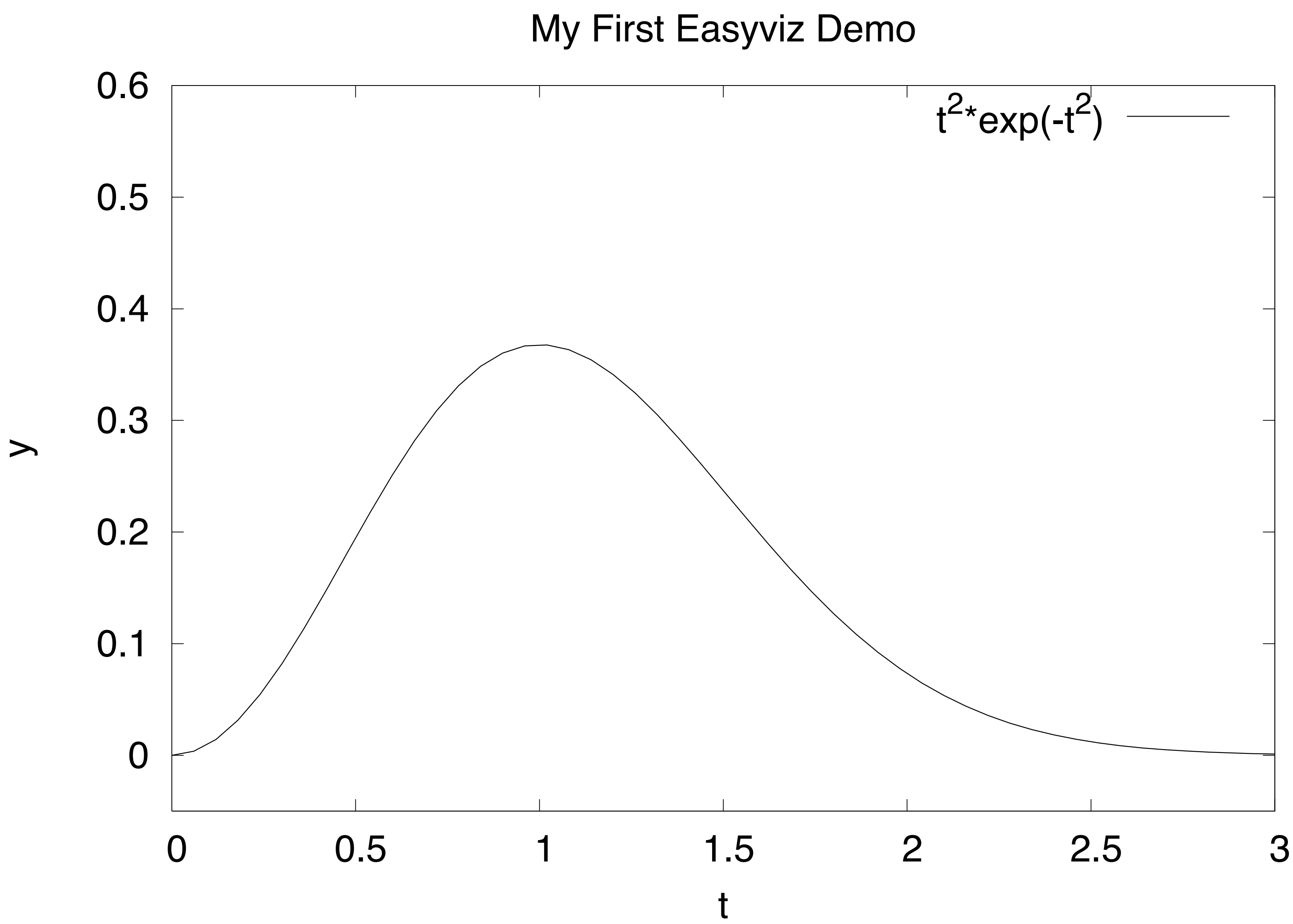
Decorating the plot

```
plot(t, y)

xlabel('t')
ylabel('y')
legend('t^2*exp(-t^2)')
axis([0, 3, -0.05, 0.6])   # [tmin, tmax, ymin, ymax]
title('My First Easyviz Demo')

# or
plot(t, y, xlabel='t', ylabel='y',
     legend='t^2*exp(-t^2)',
     axis=[0, 3, -0.05, 0.6],
     title='My First Easyviz Demo',
     hardcopy='tmp1.eps',
     show=True)   # display on the screen (default)
```

The resulting plot



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Plotting several curves in one plot

Compare $f_1(t) = t^2 e^{-t^2}$ and $f_2(t) = t^4 e^{-t^2}$ for $t \in [0, 3]$

```
from scitools.all import *   # for curve plotting

def f1(t):
    return t**2*exp(-t**2)

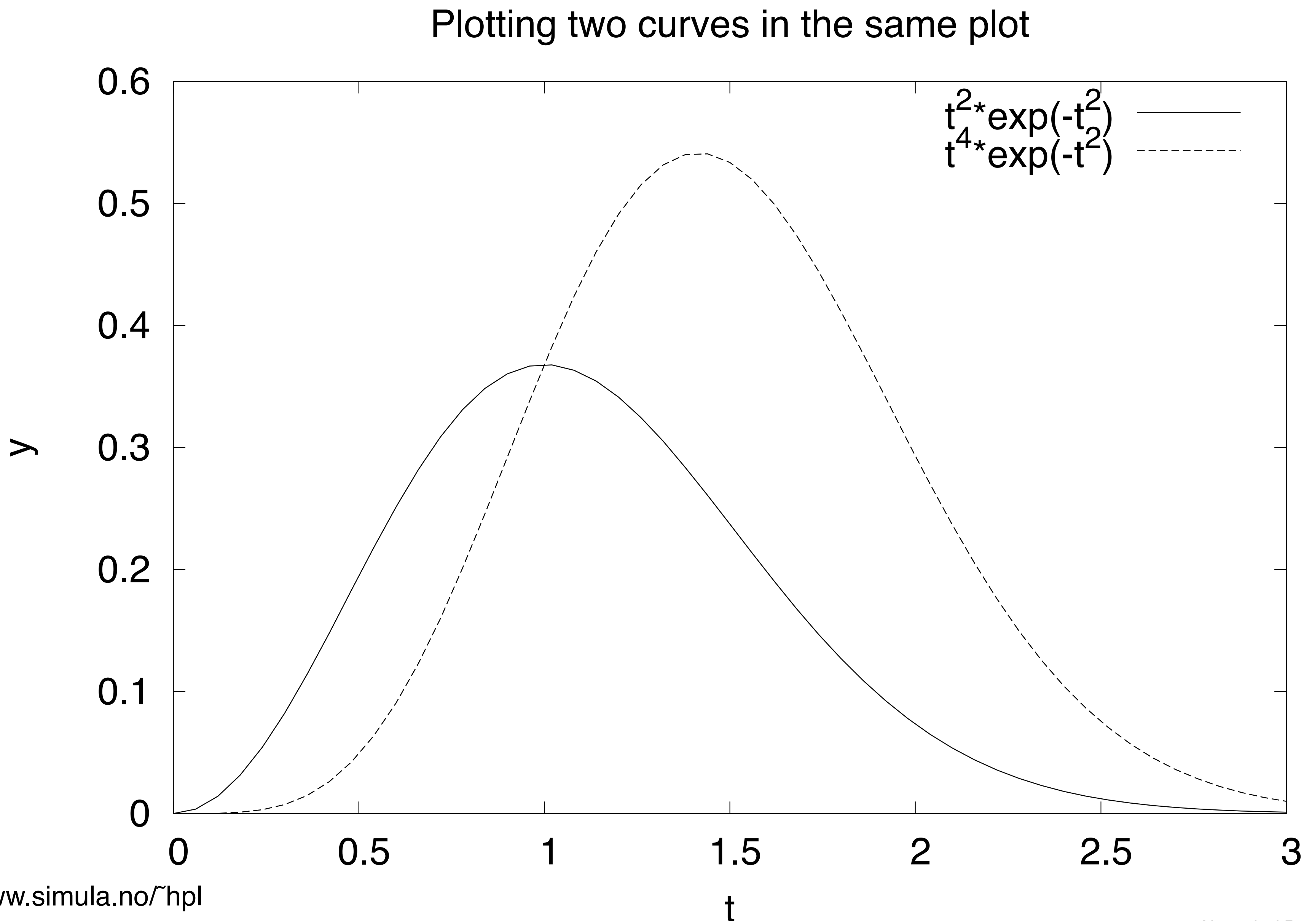
def f2(t):
    return t**2*f1(t)

t = linspace(0, 3, 51)
y1 = f1(t)
y2 = f2(t)

plot(t, y1)
hold('on')   # continue plotting in the same plot
plot(t, y2)

xlabel('t')
ylabel('y')
legend('t^2*exp(-t^2)', 't^4*exp(-t^2)')
title('Plotting two curves in the same plot')
hardcopy('tmp2.eps')
```

The resulting plot



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Example: plot a function given on the command line

- Task: plot (e.g.) $f(x) = e^{-0.2x}\sin(2\pi x)$ for $x \in [0, 4\pi]$
- Specify $f(x)$ and x interval as text on the command line:

```
Unix/DOS> python plotf.py "exp(-0.2*x)*sin(2*pi*x)" 0 4*pi
```

- Program:

```
from scitools.all import *
formula = sys.argv[1]
xmin = eval(sys.argv[2])
xmax = eval(sys.argv[3])

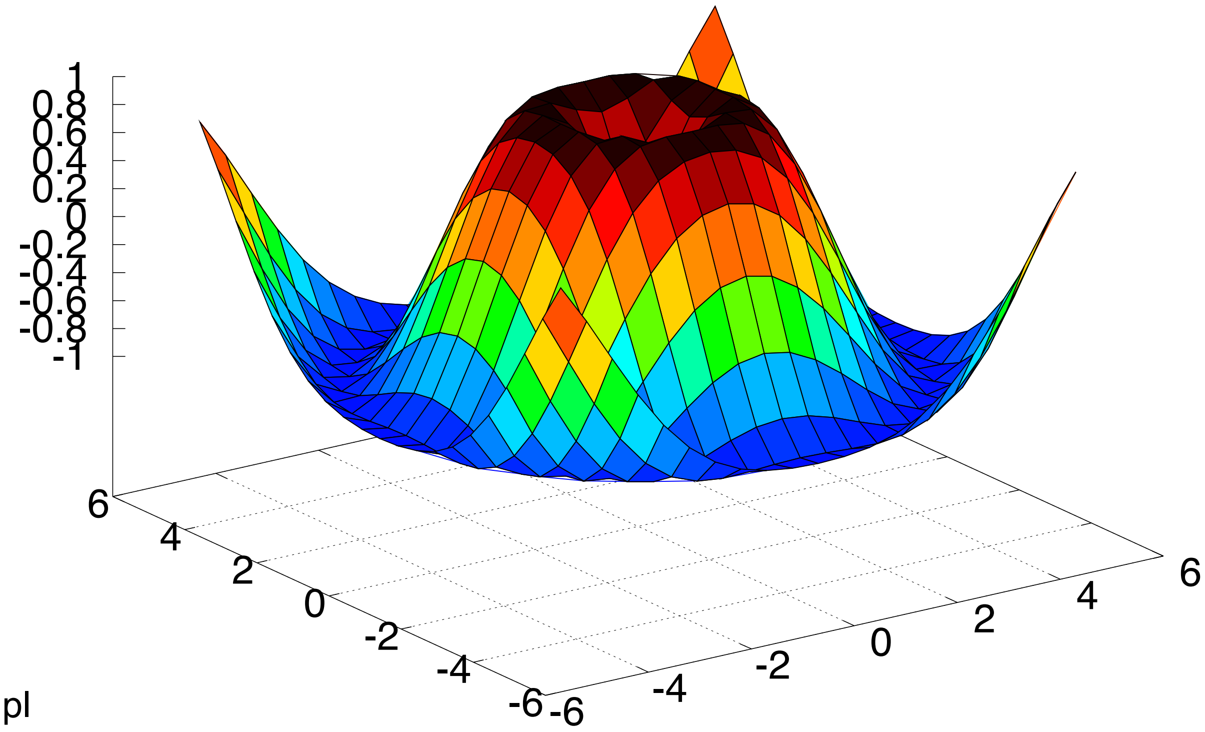
x = linspace(xmin, xmax, 101)
y = eval(formula)
plot(x, y, title=formula)
```

- Thanks to `eval`, input (text) with correct Python syntax can be turned to running code on the fly

Plotting 2D scalar fields

```
from scitools.all import *

x = y = linspace(-5, 5, 21)
xv, yv = ndgrid(x, y)
values = sin(sqrt(xv**2 + yv**2))
surf(xv, yv, values)
```



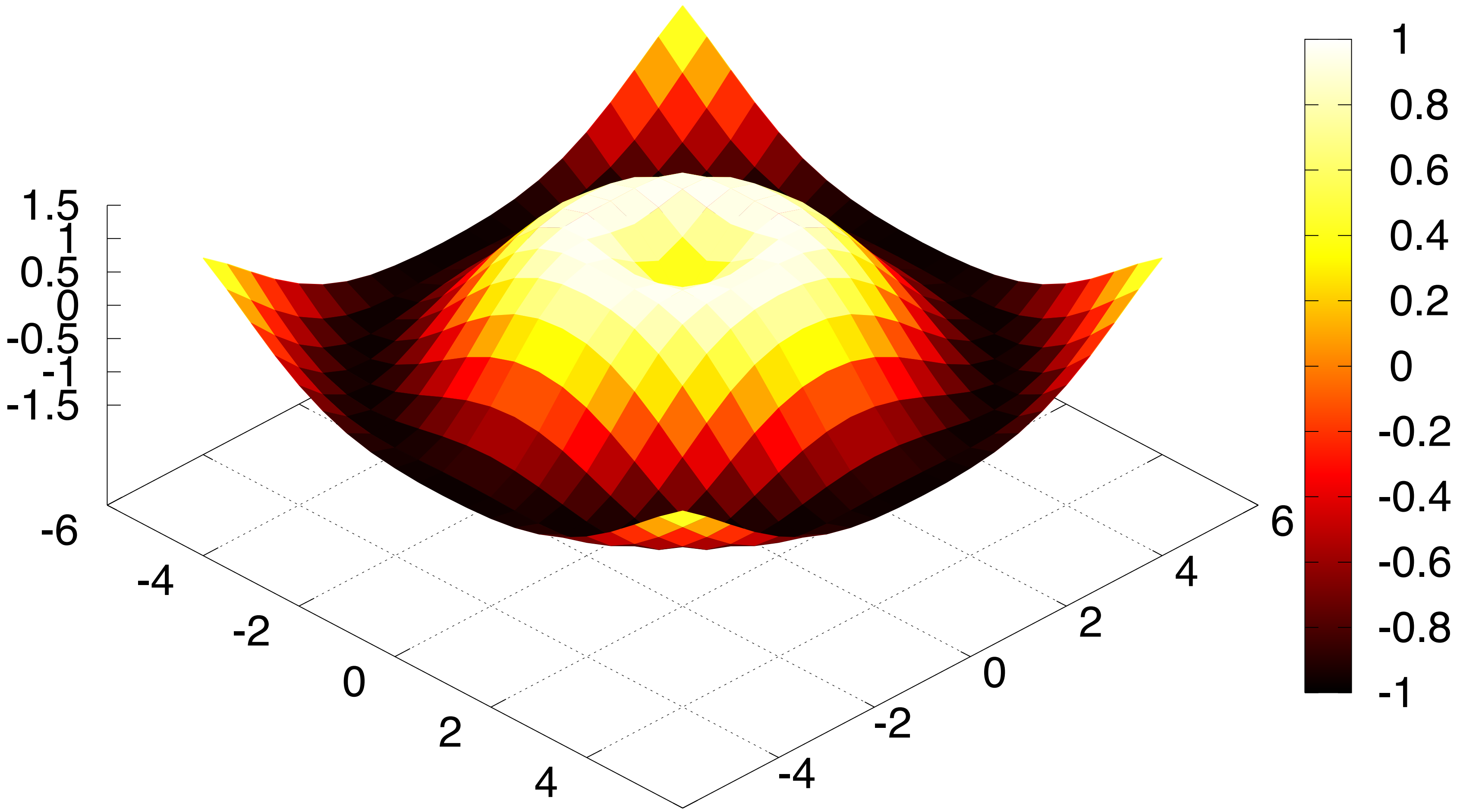
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Adding plot features

```
# Matlab style commands:
setp(interactive=False)
surf(xv, yv, values)
shading('flat')
colorbar()
colormap(hot())
axis([-6,6,-6,6,-1.5,1.5])
view(35,45)
show()

# Optional Easyviz (Pythonic) short cut:
surf(xv, yv, values,
     shading='flat',
     colorbar='on',
     colormap=hot(),
     axis=[-6,6,-6,6,-1.5,1.5],
     view=[35,45])
```

The resulting plot



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Other commands for visualizing 2D scalar fields

- `contour` (standard contours)), `contourf` (filled contours), `contour3` (elevated contours)
- `mesh` (elevated mesh), `meshc` (elevated mesh with contours in the xy plane)
- `surf` (colored surface), `surfc` (colored surface with contours in the xy plane)
- `pcolor` (colored cells in a 2D mesh)

Commands for visualizing 3D fields

Scalar fields:

- `isosurface`
- `slice_` (colors in slice plane),
  `contourslice` (contours in slice plane)

Vector fields:

- `quiver3` (arrows), (`quiver` for 2D vector fields)
- `streamline`, `streamtube`, `streamribbon` (flow sheets)

More info about Easyviz

- A plain text version of the Easyviz manual:

  `pydoc scitools.easyviz`

- The HTML version:

  `http://code.google.com/p/scitools/wiki/EasyvizDocumentation`

- Download SciTools (incl. Easyviz):

  `http://code.google.com/p/scitools/`

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